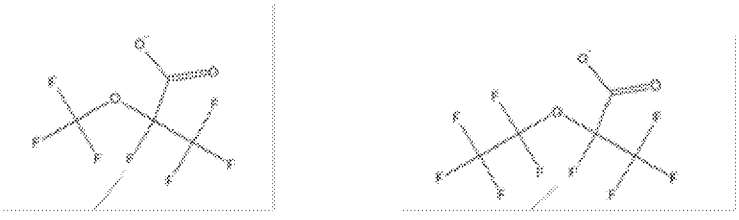
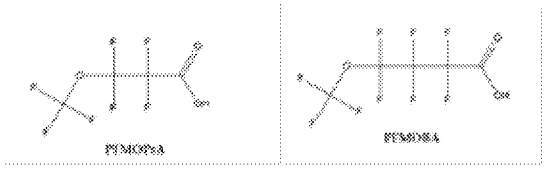
Message

From: Strynar, Mark [/O=EXCHANGELABS/OU=EXCHANGE ADMINISTRATIVE GROUP (FYDIBOHF23SPDLT)/CN=RECIPIENTS/CN=5A9910D5B38E471497BD875FD329A20A-STRYNAR, MARK]
Sent: 2/14/2017 12:44:13 PM
To: Detlef Knappe [knappe@ncsu.edu]; Lindstrom, Andrew [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=04bf7cf26aa44ce29763fbc1c1b2338e-Lindstrom, Andrew]; msun8@uncc.edu
Subject: RE: FW: Chemical Structures

In our paper Strynar et al., 2015 we proposed these structures as below: (Figure S7). These are the ones Paul suggests are more likely.



In Sun et al., 2016 we showed them different (Figure S1).



I should have noted this in the SI.

The QTOF can distinguish between the two as the likely breaking point is at the ether oxygen. We would get different fragments for the PFMOBA, not the PFMOPrA.

Mark

From: Detlef Knappe [mailto:knappe@ncsu.edu]
Sent: Monday, February 13, 2017 8:13 AM
To: Strynar, Mark <Strynar.Mark@epa.gov>; Lindstrom, Andrew <Lindstrom.Andrew@epa.gov>; msun8@uncc.edu
Subject: Re: FW: Chemical Structures

Interesting... But Synquest does make the non-branched compounds we are showing (see first two compounds in the attached). Would QTOF work be able to distinguish between linear and branched?

On 2/13/17 7:22 AM, Strynar, Mark wrote:

FYI,
I will need to take a closer look at his comment later.

Mark

From: Paul [mailto: **Personal Matters / Ex. 6**
Sent: Saturday, February 11, 2017 6:30 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Subject: Chemical Structures

Mark:

Just finishing looking at Env. Sci. & Tech. Letters 2016 3 (12) 415 for use as a reference.

Legacy and Emerging Perfluoroalkyl Substances Are Important
Drinking Water Contaminants in the Cape Fear River Watershed of
North Carolina
Mei Sun,*,†,‡ Elisa Arevalo,‡ Mark Strynar,§ Andrew Lindstrom,§ Michael Richardson,∥
Ben Kearns,∥
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⊥Town of Pittsboro, Pittsboro, North Carolina 27312, United States
#Fayetteville Public Works Commission, Fayetteville, North Carolina 28301, United States

I believe that the structural assignments for PFMOBA [$CF_3OCF_2CF_2CF_2COOH$] and PFMOPrA [$CF_3OCF_2CF_2COOH$] are most likely incorrect.

More reasonably the correct structures are isomers $CF_3CF_2OCF(CF_3)COOH$ and $CF_3OCF(CF_3)COOH$ respectively. I doubt that the MS/MS could tell the isomers apart.

If you want to discuss this further please call me. (703) 567-6832.

Best regards,

Paul

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